

String order and adiabatic continuity of Haldane chains and band insulators

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The ground state of spin-1 Haldane chains is characterized by the so-called string order. We show that the same hidden order is also present in ordinary one-dimensional band insulators. We construct a family of Hamiltonians which connects adiabatically band insulators to two topologically non-equivalent spin models, the Haldane chain and the antiferromagnetic spin-1/2 ladder. We observe that the localized spin-1/2 edge-state characteristic of spin-1 chains is smoothly connected to a surface-bound state of band insulators and its emergence is not related to any bulk phase transition. Furthermore, we show that the string order is absent in any dimensions higher than one.

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The antiferromagnetic spin-1 chain is a prominent example of a spin-liquid, an exotic state of matter where interactions play a dual role: on the one hand a strong Hund's rule coupling locally leads to the formation of magnetic spin-1 degrees of freedom, on the other hand spin correlations screen magnetism completely. As conjectured by Haldane in the early eighties¹, spin-1 chains are characterized by a finite gap in their spectrum and by exponentially decaying spin-spin correlations. Since this seminal work a lot of progress have been made, theoretically and experimentally, towards a full description of the so-called "Haldane phase". In particular, Affleck, Kennedy, Lieb and Tasaki² provided a microscopic understanding of this correlated ground state, devising an exactly solvable model (AKLT) adiabatically connected to the spin-1 chain. The AKLT ground state is made up solely of nearest-neighbor singlets (or valence bonds) and the gap in the system (and therefore in the spin-1 chain) corresponds to the energy needed to break a bond.

In this paper we want to address the question to what extent the Haldane chain is different from an ordinary band insulator. The latter has also a gap and an even number of electrons per unit cell and, recently, one of the authors has shown³ that Luttinger surfaces cannot be used to distinguish band- from correlated insulators. Two properties, though, are considered peculiar of the Haldane phase: First, when a spin-1 chain is cut, a localized fractionalized excitation, namely a spin-1/2, is formed at the boundary of the chain. These boundary spins have for example been observed in the NMR profile close to the chain ends of Mg-doped Y_2BaNiO_5 ^{4,5}. Second, the ground state possesses a hidden long-range order characterizing the entanglement of the spins: Den Nijs and Rommelse⁶ noticed that, even though true Néel order is absent in the ground state, any site with $S^z = \pm 1$ is followed by another with $S^z = \mp 1$, separated from the first by a string of $S^z = 0$ of arbitrary length. This implies that the so-called string order (SO) parameter

$$SO_{\text{chain}} = \lim_{|i-j| \rightarrow \infty} \left\langle S_i^z \exp \left(i\pi \sum_{l=i+1}^{j-1} S_l^z \right) S_j^z \right\rangle \quad (1)$$

is always finite in the Haldane phase.

A spin-1 chain can be devised on a spin-1/2 ladder using a strong ferromagnetic rung coupling J_R which binds two spin 1/2 into a single spin 1. In this case the string order parameter takes the form^{7,8,9,10}

$$SO_{\text{odd}} = - \lim_{|i-j| \rightarrow \infty} \left\langle (S_{1,i}^z + S_{2,i}^z) \exp \left(i\pi \sum_{l=i+1}^{j-1} S_{1,l}^z + S_{2,l}^z \right) (S_{1,j}^z + S_{2,j}^z) \right\rangle \quad (2)$$

and a typical ground state wave function in the Haldane phase is shown at the bottom of the first column of Fig. 1. As emphasized by Bonesteel¹¹ and Kim *et al.*⁷, this wave function has a topological feature, namely a vertical line (dashed in the figure) crosses always an *odd* number of singlets. As can be easily seen from the figure, this property is directly related to the existence of edge states at the boundaries. On the other hand, an antiferromagnetic rung coupling leads to another gapful phase, with a ground state in a different topological sector of the space of singlet wave functions. Here, always an *even* number of singlets is crossed by a vertical and edge states are absent (see Fig. 1). Correspondingly^{7,9,10} the "odd" string order SO_{odd} vanishes and instead one gets a finite "even" string order SO_{even}

$$SO_{\text{even}} = - \lim_{|i-j| \rightarrow \infty} \left\langle (S_{1,i+1}^z + S_{2,i}^z) \exp \left(i\pi \sum_{l=i+1}^{j-1} S_{1,l+1}^z + S_{2,l}^z \right) (S_{1,j+1}^z + S_{2,j}^z) \right\rangle. \quad (3)$$

In spin-ladder models these two orders never coexist as they characterize two different topological sectors.

In the following we will first show that the ground state of an ordinary band insulator can be adiabatically deformed into the ground state of either the Haldane chain or the antiferromagnetic ladder. Then we will investigate the role both of the string order and of the boundary states in the band-insulating phase. Finally, we consider the fate of the string order in dimensions larger than one.

The starting point of our discussion is the following

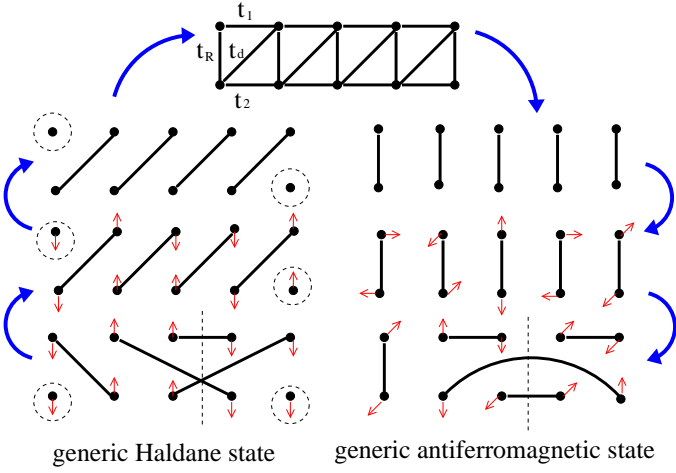


FIG. 1: Sketch of the adiabatic path connecting a generic Haldane state via a band insulator to a generic antiferromagnetic spin ladder. The two ground states in the lower two rows belong to the distinct topological sectors of the singlet spin Hilbert space as the number of singlet bonds across a vertical line (shaded) is either odd or even.

family of ladder Hamiltonians (see top of Fig. 1):

$$\begin{aligned}
 H = & \sum_{i,\alpha,\sigma} t_\alpha a_{\alpha,i,\sigma}^\dagger a_{\alpha,i+1,\sigma} + h.c. - \frac{U}{2} n_{\alpha,i,\sigma} \\
 & + \sum_{i,\sigma} t_R a_{1,i,\sigma}^\dagger a_{2,i,\sigma} + t_D a_{1,i+1,\sigma}^\dagger a_{2,i,\sigma} + h.c. \\
 & + U \sum_{i,\alpha} n_{\alpha,i,\uparrow} n_{\alpha,i,\downarrow} + J_R \sum_i \mathbf{S}_{1,i} \mathbf{S}_{2,i} \quad (4)
 \end{aligned}$$

where α indicates the two legs of the ladder (or two orbitals of an atom). Varying the set of parameters $[t_1, t_2, t_R, t_D, U, J_R]$, it is possible to span a rich phase diagram including a Mott-insulating Haldane phase ($U \gg t_i, J_R + t_R^2/U < 0$), an antiferromagnetic ladder ($U \gg t_i, J_R = 0$) and band-insulators ($U = 0, J_R = 0$). We now describe how these states can be connected adiabatically following the route depicted in Fig. 1. First, it has been shown both numerically^{8,9,10} and using analytic arguments^{7,12} that the Haldane chain can be adiabatically deformed into a spin-1/2 model with only diagonal antiferromagnetic couplings, and, similarly, the antiferromagnetic ladder is connected to a pure rung singlet model (second last row of Fig. 1). These local antiferromagnets can be realized as the large U limit of the two-sites Hubbard Hamiltonian

$$\begin{aligned}
 H_{\text{loc}} = & \sum_\sigma t(c_{1,\sigma}^\dagger c_{2,\sigma} + h.c.) - \frac{U}{2}(n_{1,\sigma} + n_{2,\sigma}) \\
 & + U(n_{1,\uparrow} n_{1,\downarrow} + n_{2,\uparrow} n_{2,\downarrow}) \quad (5)
 \end{aligned}$$

for the diagonal or the rung, respectively. For arbitrary U/t , the three lowest eigenvalues of H_{loc} are a singlet with energy $E_s = -\frac{1}{2}(U + \sqrt{U^2 + 16t^2})$, a triplet with

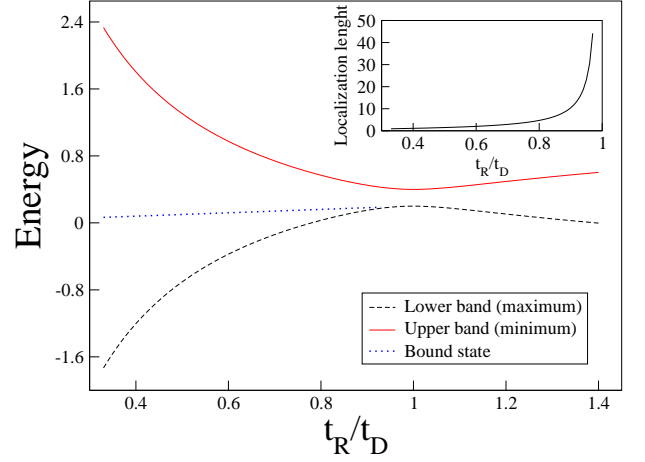


FIG. 2: Energy of the bound state compared to the maximum (minimum) of the upper (lower) band as a function of t_R/t_D ($t_1 = -0.1, t_2 = -0.2$ and $t_R = -1$). In the inset the localization length of the bound state is shown.

$E_t = -U$ and a charge excitation with $E_c = -\frac{U}{2} - |t|$. The gap

$$\Delta = \frac{1}{2} \min \left[\sqrt{U^2 + 16t^2} - U, \sqrt{U^2 + 16t^2} - 2|t| \right] \quad (6)$$

is always finite and, therefore, one can switch off the interaction U completely, connecting adiabatically the Mott- and the band-insulating ground states. Note that the nature of the lowest excitation changes completely when $E_c = E_1$ while the ground state rotates smoothly³ from a state describing two localized spins to one where two electrons occupy the bonding band.

As a final step, we have to show that these two local insulators can be adiabatically connected in the non-interacting limit, $U, J_R = 0$ where the band-structure is given by

$$\begin{aligned}
 E^{1,2} = & (t_1 + t_2) \cos(ka) \pm [(t_1 - t_2)^2 \cos^2(ka) + \\
 & (t_R - t_D)^2 + 2t_R t_D (1 + \cos(ka))]^{1/2}. \quad (7)
 \end{aligned}$$

The states in the second row of Fig. 1 are described by $t_1, t_2, t_R = 0$ and $t_1, t_2, t_D = 0$, respectively. For $2|t_1 + t_2| < |t_D + t_R| + |t_D - t_R|$ and $t_1 \neq t_2$, the state is always a band insulator with a finite gap. Therefore by reducing t_D and increasing t_R for finite $t_1 - t_2$ we can complete the adiabatic path of Fig. 1. For $t_1 = t_2$ the Hamiltonian of Eq. (4) has a quantum critical point at $t_R = t_D$ (related to an extra particle-hole symmetry of this model). In Fig. 2 we show that for small $t_1 - t_2$ the gap remains finite upon tuning from the diagonal to the rung insulator.

After having shown the adiabatic continuity, we consider now the evolution of the string order along the adiabatic path. In Eqns. (2) and (3) the $S_{1-2,i}^z$ were operators living in the spin Hilbert space while for the Fermionic model we have to replace those by $S_{1-2,i}^z = \frac{1}{2}(n_{1-2,i,\uparrow} - n_{1-2,i,\downarrow})$. For the two local singlet states of the third row

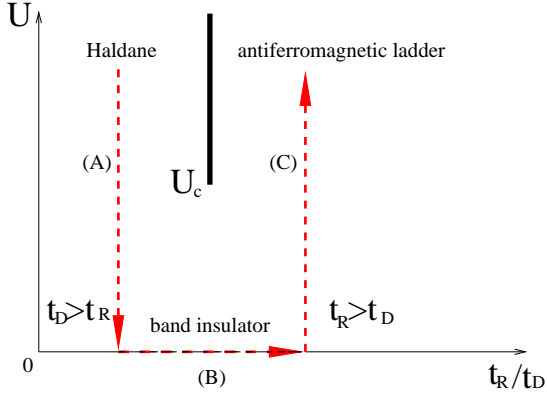


FIG. 3: Schematic phase diagram of the generalized Hubbard ladder (4). The dashed lines denote the adiabatic path of Fig. 1. For sufficiently large interactions, either a second or first order transition or new intervening phases are expected.

of Fig. 1 the string order is maximal⁷, with $SO_{\text{odd}} = \frac{1}{4}$, $SO_{\text{even}} = 0$ and $SO_{\text{even}} = \frac{1}{4}$, $SO_{\text{odd}} = 0$, respectively. Remarkably, the string order is also finite for the two local band insulators of the second row: $SO_{\text{odd}} = \frac{1}{16}$, $SO_{\text{even}} = 0$ and $SO_{\text{even}} = \frac{1}{16}$, $SO_{\text{odd}} = 0$, respectively. The factor 4 reduction arises because empty and doubly occupied states appear with a probability of 1/2, affecting the spin operators at the beginning and at the end of the string. The string, however, still contributes with a factor 1. How can these different "order parameters" be connected? To answer this question we calculate the two string orders along the adiabatic path connecting the two local insulators (i.e. on segment B of Fig. 3). With the help of the identities $e^{ac^\dagger c} = e^{(e^\alpha - 1)c^\dagger c}$: and $S_i^z = -\frac{1}{4} (: e^{-2c_{i,\uparrow}^\dagger c_{i,\uparrow}} : - : e^{-2c_{i,\downarrow}^\dagger c_{i,\downarrow}} :))$ where $: \dots :$ denotes normal ordering, we can reformulate Eq. (2) as

$$SO_{\text{odd}}(i, j) = \langle \frac{1}{16} : \sum_{r,l=1,2} (e^{-2n_{r,i,\uparrow}} - e^{-2n_{r,i,\downarrow}}) \times \exp\left(\sum_{\substack{k=i+1 \\ s=1,2}}^{k=j-1} (-1+i)n_{s,k,\uparrow} + (-1-i)n_{s,k,\downarrow}\right) \times (e^{-2n_{l,j,\uparrow}} - e^{-2n_{l,j,\downarrow}}) : \rangle \quad (8)$$

and a similar expression is valid for Eq. (3). In analogy to the string order in the spin sector one can also introduce a similar quantity in the charge sector, see Appendix A.

For a non-interacting system, one can easily evaluate expectation values of the form $\langle : e^{c_i^\dagger A_{ij} c_j} : \rangle = \text{Det}[1 + G \cdot A]$ using functional integration, where G is the equal-time Greens function matrix. We therefore obtain

$$SO_{e/o}^z(i, j) = \frac{1}{16} \sum_{\substack{\alpha, \beta = \uparrow, \downarrow \\ r, k = 1, 2}} (-1)^{2+\delta^{\alpha, \beta}} \text{Det}[I + G \cdot A_{e/o}^{r, i, \alpha, k, j, \beta}], \quad (9)$$

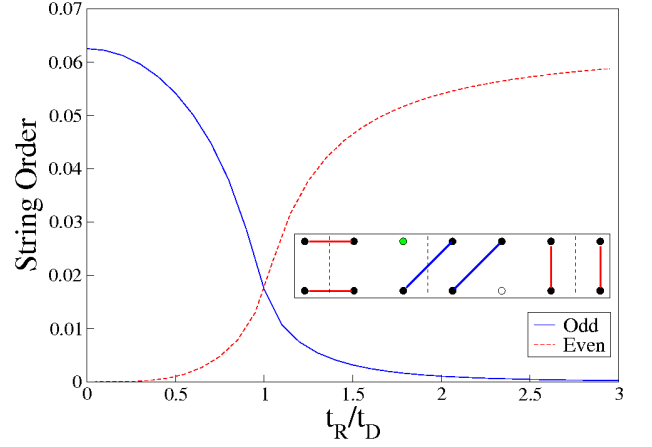


FIG. 4: The even and odd string orders, SO_{even} and SO_{odd} , for the non-interacting ladder as a function of t_R/t_D ($t_1 = -0.1$, $t_2 = -0.2$, $t_R = -1$). Inset: in the presence of charge fluctuations a vertical line can cross both even and odd number of singlets. Accordingly the two string orders can coexist.

where the matrices $A_{e/o}$ can be read off from Eq. (8) and the G matrix can easily be obtained numerically for arbitrary t_1, t_2, t_R, t_D . Also the determinant in Eq. (9) can be easily computed for large systems and the SO parameters are obtained from the limit $|i - j| \gg \xi$, where $\xi \propto 1/\Delta$ is the correlation length.

We find that in one-dimensional band insulators string order is always present – even in the absence of interactions! In contrast to the pure spin models generically both string order parameters are finite (see Fig. 4) and they are smooth functions of t_R/t_D for $t_1 \neq t_2$. In our model, for $t_R = t_D$ the two string orders are equal by symmetry, $SO_{\text{even}} = SO_{\text{odd}}$ (this follows from the more general relation $SO_{\text{even}}(t_R, t_D, t_1, t_2) = SO_{\text{odd}}(t_D, t_R, t_2, t_1)$ that can be understood in terms of the following transformation on the ladder: shift of the lower leg by one lattice site and mirror-reflection of the ladder respect the x-axis). Only for $t_1 = t_2$ and $t_R = t_D$, when the gap vanishes, both SO_{even} and SO_{odd} deplete to 0 because at the critical point singlets of arbitrary length are generated. The two orders, SO_{odd} and SO_{even} , coexist in gapped insulators also in the presence of strong interactions as long as (virtual) charge fluctuations are allowed. This can be seen from the inset of Fig. 4: a doubly occupied or empty site allows to switch from diagonal to rung singlets.

We now outline the consequences of our discussion for the phase diagram of generalized Hubbard ladders, sketched in Fig. 3. First, gapped systems are stable against small perturbations and therefore there is a finite range of parameters which allows to connect adiabatically Haldane states and antiferromagnetic ladders. Second, in a pure spin model it is *not* possible to connect these two phases as their wave functions live in different topological sectors of the spin Hilbert space. Therefore, we expect that beyond some critical value of U a phase

transition line (first or second order) or an intervening phase should separate the even and odd sectors^{7,13,14,15}.

For pure spin models, Strykh and Balents¹³ analyzed the possible intervening phases and concluded that without extra fine-tuning there is never a direct second order transition from the Haldane to the antiferromagnetic ladder. Either the transition is first order or intervening phases with broken translational invariance appear. The absence of a direct second-order transition is consistent with our finding that the two high-symmetry phases are adiabatically connected.

To gain further insight in nature of the phase diagram sketched in Fig. 3 at finite U , we observe that for $t_R = t_D$ and $J_R = 0$, our ladder gains an extra mirror symmetry (this is evident unfolding the ladder on a chain, as shown in the lower part of Fig. 5) and we expect that its properties are similar to the ones of the well-studied^{15,16,17,18} one-dimensional *ionic* Hubbard model (i.e. a Hubbard model with a staggered potential) which has the same symmetries. For this system upon increasing U (see upper part of Fig. 5) first the charge gap of the band insulator closes and one obtains a dimerized phase for $U_{c1} < U < U_{c2}$. For $U > U_{c2}$ the system becomes a uniform, gapless Mott insulator (effectively a uniform Heisenberg *chain*¹⁸). We therefore expect that U_c in the schematic phase diagram of Fig. 3 has a similar role as U_{c1} , i.e. the charge gap vanishes and a dimerized phase (not shown in Fig. 3) appears for $U > U_{c1}$, $t_R \sim t_D$, where SO_{even} is bigger or smaller than SO_{odd} , depending on which of the two degenerate ground states one considers. According to the results of Strykh and Balents¹³ discussed above, we do, however, not expect a gapless phase for generic parameters (e.g. $J_R > 0$). The role of string order in the charge sector of the ionic Hubbard model is briefly discussed in Appendix A.

At this point we would like to investigate the emergence of the edge-states following again the path depicted in Fig. 1. The localized spin 1/2 at the boundary of the Haldane phase evolves smoothly in a surface bound state of the "diagonal" band insulator. For finite interactions and a proper choice of the chemical potential, this surface bound state will be singly occupied giving rise to a localized spin. In Fig. 2 we show how this edge state merges with one of the bands when t_R is increased for $t_1 \neq t_2$. At this point, the localization length of this state diverges with $(t_R/t_D - \text{const.})^{-1}$ (inset of Fig. 2). Nevertheless, this is not related to any bulk phase transition.

Up to now we have only discussed one-dimensional ladders and it is interesting to study the role of string order in higher dimensions. Especially in gapped systems one would naively expect that any type of long-range order is stable against small perturbations like a coupling to neighboring ladders. Using the methods described above, we can easily calculate the string order for two- and three-dimensional band insulators numerically. Surprisingly we find that for arbitrarily weak inter-ladders coupling, t_\perp , the string order decays exponentially, $SO(i, j) \sim e^{-\alpha|i-j|}$

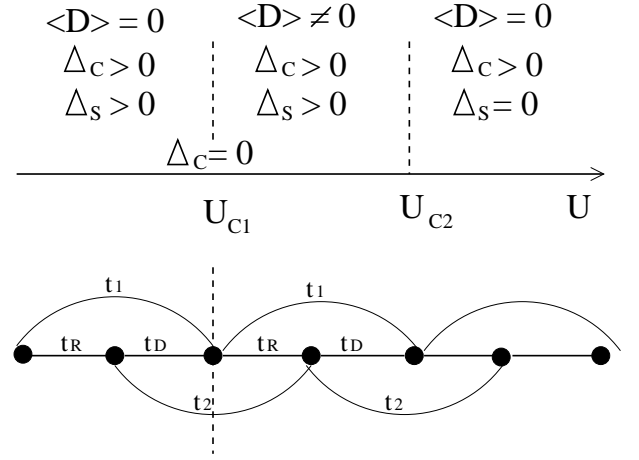


FIG. 5: Top: the three different phases of the ionic Hubbard model as a function of U . Δ_c and Δ_s are the charge and spin gaps and $D = \frac{1}{L} \sum_{j,\sigma} (-1)^j \langle c_{j+1,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{j+1,\sigma} \rangle$ is the dimerization order parameter^{15,16}. Bottom: the ladder of Eq. (4) unfolded on a chain. An extra mirror symmetry is present for $t_R = t_D$ and $J_R = 0$.

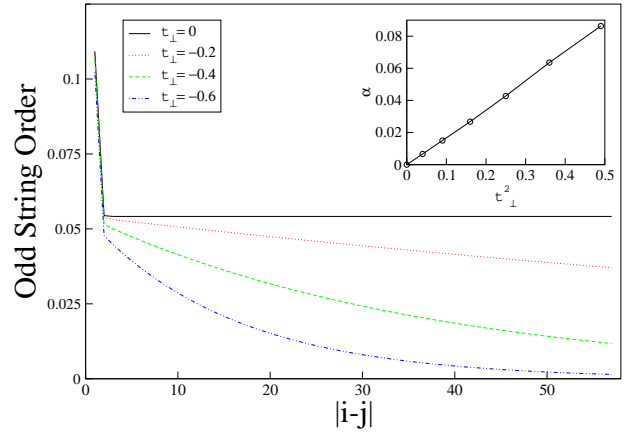


FIG. 6: The odd string order of Eq. (9) for a two-dimensional lattice decays as $SO_{\text{odd}} \approx e^{-\alpha|i-j|}$ (with $t_1 = -0.1$, $t_2 = -0.2$, $t_R = -1$, $t_D = -2$ and $t_\perp = 0, -0.2, -0.4, -0.6$ from up to down). Inset: α as a function of t_\perp^2 .

with $\alpha \propto t_\perp^2$ (see Fig. 6). A similar observation has been made previously by Todo *et al.*¹⁹, who studied spin-1 ladders numerically. The decay of the string order is a consequence of (rare) inter-ladders singlets which introduce a random phase $e^{\pm i\pi/2}$ in the string. We note that obvious generalizations¹⁹ of the string order parameter to higher dimensions (replacing strings by squares or cubes) are ineffective again due to "dangling singlets" at the infinite surface of such structures.

In conclusions, we have shown that three phases with both spin- and charge gaps and two electrons per unit cell, namely Haldane chains, band-insulators and antiferromagnetic ladders, are actually all the same in the sense that their unique ground states can be adiabatically connected (the excitation spectra, however, may

change). This cousinship is reflected in the prevalence of string order in all these one-dimensional phases, even in non-interacting band insulators. However, string order is not robust in higher dimensions, where it is destroyed by arbitrarily weak coupling²⁰. An interesting open question is the precise role of the Schrieffer-Wolff transformation, a central tool to derive effective models. Such a unitary transformation eliminates charge degrees of freedom completely and therefore maps the non-magnetic ground state of Hamiltonians with charge gap into one of the topological sectors of the spin models. As we have connected two *different* sectors adiabatically along our path, this seems to imply that the Schrieffer-Wolff transformation has to break down at some point. This is consistent with a scenario where at U_c in Fig. 3 the charge gap closes. However, one also has to take into account that a Schrieffer-Wolff transformation is not uniquely defined as it depends e.g. on the choice of a single-particle basis and therefore the topological sector may not be uniquely defined in the presence of charge fluctuations.

The rapid progress in the control of fermionic atoms in optical lattices will make possible to study the adiabatic evolution of correlated ground states also experimentally in the near future^{21,22}.

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APPENDIX A: CHARGE STRING ORDER IN BAND- AND MOTT-INSULATORS

In close analogy with the case of the spins (Eqns. (2) and (3) in the text), we can construct string order parameters also in the charge sector. We define SO_{even}^c and SO_{odd}^c as

$$SO_{\text{odd}}^c = \lim_{|i-j| \rightarrow \infty} \left\langle (\delta n_{1,i} + \delta n_{2,i}) \exp \left(i \frac{\pi}{2} \sum_{l=i+1}^{j-1} \delta n_{1,l} + \delta n_{2,l} \right) (\delta n_{1,j} + \delta n_{2,j}) \right\rangle \quad (\text{A1})$$

$$SO_{\text{even}}^c = \lim_{|i-j| \rightarrow \infty} \left\langle (\delta n_{1,i+1} + \delta n_{2,i}) \exp \left(i \frac{\pi}{2} \sum_{l=i+1}^{j-1} \delta n_{1,l+1} + \delta n_{2,l} \right) (\delta n_{1,j+1} + \delta n_{2,j}) \right\rangle \quad (\text{A2})$$

where $\delta n_i = n_{i,\uparrow} + n_{i,\downarrow} - \langle n_{i,\uparrow} + n_{i,\downarrow} \rangle$.

As shown in Fig. 7, both SO_{odd}^c and SO_{even}^c are finite for a generic band insulator and - up to a trivial factor 1/4 - very similar (but not identical) to the spin string order parameters of Fig. 4. In the purely diagonal ($t_R = 0$) and vertical ($t_D = 0$) limits only one of the two string orders is different from 0.

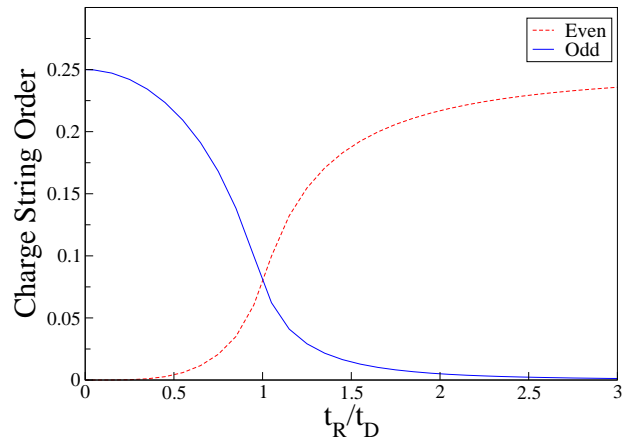


FIG. 7: SO_{odd}^c and SO_{even}^c as a function of t_R/t_D for the set of parameters $t_1 = -0.1$, $t_2 = -0.2$ and $t_R = -1$.

The presence of charge string order comes as a natural consequence of the symmetry existing in the one-dimensional band insulator between the spin and the charge sectors. In bosonization language, both the spin and charge fields are pinned due to the presence of a relevant cosine term in the low energy Bosonic Hamiltonian²³, leading therefore to finite string order parameters^{7,20}. As already discussed in the main text, this scenario is stable also in presence of interactions (at least for truly one-dimensional systems), as long as both the Bosonic fields are massive. In the limit of large U , the charge string orders will be strongly suppressed by powers of $1/U$ due to the smallness of the charge fluctuations (becoming strictly zero for a pure spin model, i.e. $U = \infty$) but will remain finite for any finite U .

In the case of the ionic Hubbard model (corresponding to the higher symmetry manifold $t_R = t_D$ and $J_R = 0$ in the parameter space of Eq. (4)) the charge field becomes massless at $U = U_{c1}$ due to the competition between two relevant cosine perturbations¹⁵ (the on-site energy and the Coulomb interaction). As both for $U < U_{c1}$ and $U > U_{c1}$ the charge field is locked, the charge string order will be finite but it will vanish at the gapless point $U = U_{c1}$ (the spin string order stays finite at U_{c1}).

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